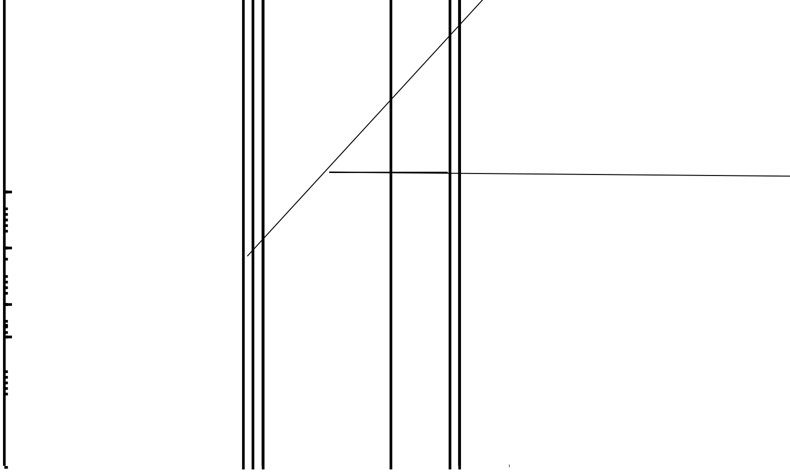
$$V(r,r') = \alpha\sum_i \frac{\psi_i(r) \quad (\mu|r \quad r'|)\psi_j^*(r)}{|r \quad r'|}. \qquad (2)$$

A a a a a a $\mu$=0.2 [1] a a a-
a .[15] T PBE a
$\mu$=0 E . (2). S a a HF
a HSE a a a ,
a $\alpha$ a PBE a
0.25, a a a ~0.40 a
a a Z O.[16] W a (HSE-25/HSE-40)
a . F 1
a X a DFT a ,
a a a HF a
a a ($r$ $r'$). T a
a a -
, a , a a Z O.[12,16 21]
H , a a HF-DFT a
HF a (F . 1) a Z O,
a a a a a
a a a
a . T a a
a a a a a
a , a
LDA. T a -
a LDA- a
Z O,[9,22]

a a ( X, PBE , HSE-25, a HSE-40) Ta II,
a a GGA ( )



4( ) X a a a a $V_Z$ . I a . T - a a .[31,32] E LDA+*U* a .[22] O a , a $V_O$ a a a Z , F . 4(a) 4( ).

### E. Assessment of previous LDA-corrected calculations

T a a a -LDA X, HSE, GW a a LDA- , a - . W GGA-C (C=C ). E a LDA+*U* Ja a Va Wa[22] a a , a a *U* Z 3*d* a a , a a . La[9] - a a *U* (=6 V) $E_V$ 0.7 V, a - a a (CBM). T a LDA-C a a . W a a a a -LDA a a , : ( ) F . 5 a Ta II a X a $V_O$ a a LDA-C . T

a $V^0$ +0.85 V X a +1 V HSE a La[9] a a 1.0 V O a.[16] I a 4 V Ja .[22] T +0.85 V a a a a $10^{19}$ $^3$ a 700 C, - .[28]

( ) T a a (0/++) $V_O$ : HSE-40 a X, a a a $E_V$ +(2.2 2.3) V, Ja [22] I a , a HSE-25 a $E_V$+1.7 V, GW a a HSE-25 (R . 23) $E_V$+1.7 V 1.4 V (GW GGA+*U*). T a LDA+C La [9] a a (0/++) a $E_V$ +1.3 V.

*J @ . a .a .

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